New approximate radial wave functions
for power-law potentials

Vladimir Kudryashov*

B.I. Stepanov Institute of Physics,
National Academy of Sciences of Belarus,
68 Nezavisimosti Ave., 220072 Minsk, Belarus

Radial wave functions for power-law potentials are approximated with the help of power-law substitution and explicit summation of the leading constituent WKB series. Our approach reproduces the correct behavior of the wave functions at the origin, at the turning points and far away from the turning points

I. INTRODUCTION

Many interesting physical problems require solving the Schrödinger equation for spherically symmetric potentials $V(r)$. The separated radial Schrödinger equation can be written in the form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(r)}{dr^2} + (V(r) + V_c(r) - E)\,\psi(r) = 0 \qquad (1)$$

which is identical to the one-dimensional Schrödinger equation with an effective potential given by the sum of the origin potential $V(r)$ and the centrifugal potential

$$V_c(r) = \frac{\hbar^2 l(l+1)}{2mr^2}. \qquad (2)$$

In the present work we consider power-law potentials

$$V(r) = \alpha r^k, \quad \alpha > 0, \quad k \geq 1 \qquad (3)$$

which are very important in particle physics. It is known that only several potentials permit the exact solutions of the Schrödinger equation. Usually realistic physical calculations are impossible without different approximation techniques. One of the earliest and simplest methods of obtaining approximate eigenvalues and eigenfunctions of the radial Schrödinger equation is the WKB method (see, e.g., [1, 2] and references therein).

It is known [1, 3] that a suitable transformation of the initial equation improves results of an approximation technique. We examine the power-law substitutions

$$r = q^s, \quad s > 0, \quad \psi(r) = r^{(s-1)/2s}\Psi(q). \qquad (4)$$

The transformed equation is

$$-\hbar^2\frac{d^2\Psi(q)}{dq^2} + Q(q)\Psi(q) = 0 \qquad (5)$$

*Electronic address: kudryash@dragon.bas-net.by

where

$$Q(q) = \frac{2ms^2}{q^2}\left(\alpha q^{(2+k)s} - Eq^{2s}\right)$$
$$+ \frac{\hbar^2}{q^2}\left(s^2(l+1/2)^2 - \frac{1}{4}\right). \qquad (6)$$

Of course, the exact solutions do not depend on some substitution. However, we are interesting in the approximate solutions. R. E. Langer [1] has used the particular case $s = 2$ when he was applying the WKB approximation to the Kepler problem.

The WKB approach deals with the logarithmic derivative

$$Y(q) = \frac{d\ln\Psi(q)}{dq} \qquad (7)$$

that satisfies the nonlinear Riccati equation

$$-\hbar^2\left(\frac{dY(q)}{dq} + Y^2(q)\right) + Q(q) = 0 \qquad (8)$$

where $Q(q)$ is an arbitrary function of q (naturally not only the special expression (6)). The WKB series

$$Y_{as}^{\pm}(q) = \hbar^{-1}\left(\pm Q^{1/2} + \sum_{n=1}^{\infty}\hbar^n Y_n^{\pm}(q)\right) \qquad (9)$$

are the asymptotic expansions in powers of Plank's constant $\hbar$ of two independent particular solutions of the Riccati equation. The usual WKB approximations

$$Y_{WKB}^{\pm}(q) = \hbar^{-1}\left(\pm Q^{1/2} + \sum_{n=1}^{N}\hbar^n Y_n^{\pm}(q)\right)$$

contain a finite number of leading terms $Y_n^{\pm}(q)$ from the complete expansions $Y_{as}^{\pm}(q)$. These approximations are not valid at the turning points where $Q(q) = 0$ and at the origin $q = 0$. While in most cases of improvements of the WKB method (see, e.g., [2, 3, 4, 5]) the main purpose is to achieve highest accuracy in eigenvalue calculation for the radial Schrödinger equation, our goal is to construct satisfactory approximate eigenfunctions with the correct behavior at the origin, at the turning points and far away from the turning points.

II. NEW APPROXIMATIONS FOR LOGARITHMIC DERIVATIVES

The analysis of the well-known structure of the leading $Y_n^{\pm}(q)$ and recursion relations [6, 7] allows us to reconstruct the asymptotic WKB series as the infinite sums

$$Y_{as}^{\pm}(q) = \pm\hbar^{-1}Q^{1/2} + \sum_{j=1}^{\infty} Z_{as,j}^{\pm}(q) \qquad (10)$$

of new constituent (partial) asymptotic series $Z_{as,j}^{\pm}(q)$ [8, 9].

The complete series $Y_{as}^{\pm}(q)$ are approximated by a finite number of leading constituent series $Z_{as,j}^{\pm}(q)$ in contrast to the use of a finite number of leading terms $Y_n^{\pm}(q)$ in the conventional WKB approach. Using notation

$$a(q) = \frac{1}{\hbar^{2/3}} \frac{Q(q)}{|dQ(q)/dq|^{2/3}}, \qquad (11)$$

$$b_1(q) = \frac{1}{\hbar^{2/3}} \frac{dQ(q)/dq}{|dQ(q)/dq|^{2/3}}, \qquad (12)$$

$$b_2(q) = \frac{d^2Q(q)/dq^2}{dQ(q)/dq} \qquad (13)$$

we are able to rewrite two first leading constituent series in the form

$$\begin{aligned} &\pm \hbar^{-1}Q^{1/2} + Z_{as,1}^{\pm}(q) + Z_{as,2}^{\pm}(q) \\ &= b_1(q)y_{as,1}^{\pm}(a) + b_2(q)y_{as,2}^{\pm}(a). \end{aligned} \qquad (14)$$

Direct verification shows that the series $y_{as,1}^{\pm}(a)$ and $y_{as,2}^{\pm}(a)$ satisfy equations

$$\frac{dy_{as,1}^{\pm}}{da} + (y_{as,1}^{\pm})^2 = a, \qquad (15)$$

$$\frac{dy_{as,2}^{\pm}}{da} + 2y_{as,1}^{\pm}y_{as,2}^{\pm} = \frac{1}{3}\left(2a\frac{dy_{as,1}^{\pm}}{da} - y_{as,1}^{\pm}\right). \qquad (16)$$

Eq.(15) is the Riccati equation for the logarithmic derivatives of linear combinations of the well-studied Airy functions $\mathrm{Ai}(a)$ and $\mathrm{Bi}(a)$ [10] .

The particular expressions

$$y_1^{\pm}(a) = \frac{d}{da}\ln\left(\mathrm{Ai}(a) \pm i\mathrm{Bi}(a)\right),$$

$$y_1^-(a) = \frac{d}{da}\ln\mathrm{Ai}(a), \quad y_1^+(a) = \frac{d}{da}\ln\mathrm{Bi}(a)$$

correspond to the conventional WKB series .

Generalization consists in the use of formulas

$$y_1(a;t) = \frac{d}{da}\ln\left(\mathrm{Ai}(a) + t\mathrm{Bi}(a)\right), \qquad (17)$$

$$y_2(a;t) = \frac{1}{30}\left[-8a^2(y_1(a;t))^2 - 3 - 4ay_1(a;t) + 8a^3\right] \qquad (18)$$

with a mixture parameter t. As a result we get new approximate logarithmic derivative

$$Y_{app}(q) = Y(q;t) = b_1(q)y_1(a;t) + b_2(q)y_2(a;t) \qquad (19)$$

which satisfies the following equation

$$\begin{aligned} &-\hbar^2\left(\frac{dY(q;t)}{dq} + Y^2(q;t)\right) + Q(q) = -\hbar^2\left[\left(\frac{d^3Q(q)/dq^3}{dQ(q)/dq}\right)y_2(a;t)\right. \\ &\left. + \left(\frac{d^2Q(q)/dq^2}{dQ(q)/dq}\right)^2\left(y_2^2(a;t) - \frac{8}{3}y_2(a;t) + \frac{4}{3}ay_1(a;t)y_2(a;t) - \frac{1}{6}\right)\right] \end{aligned} \qquad (20)$$

instead of Eq. (8).

It is not surprising that the asymptotics of our approximation coincide with the WKB asymptotics far away from the turning points. At the same time our approximation reproduces the known [7] satisfactory approxima-

tion near the turning points.

III. NEW APPROXIMATIONS FOR WAVE FUNCTIONS

Now we can construct the approximate radial wave functions for the bound states in the case of a power-law potential when $Q(q)$ is of the form (6).

First, we must reproduce the correct limiting behavior at the origin. In this case we have the following exact expressions $(r \to 0, q \to 0)$

$$\psi_{ex}(r) \to r^{l+1}, \quad \Psi_{ex}(q) \to q^{sl+(s+1)/2},$$

$$Y_{ex}(q) \to \frac{sl+(s+1)/2}{q}. \tag{21}$$

At the same time we can derive relations

$$a(q) \to a_0 = \left(\frac{s^2}{4}(l+1/2)^2 - \frac{1}{16}\right)^{1/3},$$

$$b_1(q) \to -\frac{2a_0}{q}, \quad b_2(q) \to -\frac{3}{q},$$

$$Y(q;t) \to -\frac{1}{q}(2a_0 y_1(a_0;t) + 3y_2(a_0;t)) \tag{22}$$

in the framework of our approach. We obtain the algebraic equation for determining the value of t. Its solution is

$$t_0 = \frac{-c(l,s)\mathrm{Ai}(a_0) + a_0(d\mathrm{Ai}(a_0)/da_0)}{c(l,s)\mathrm{Bi}(a_0) - a_0(d\mathrm{Bi}(a_0)/da_0)} \tag{23}$$

where

$$c(l,s) = 1 - \sqrt{1 + \frac{5}{4}\left(\frac{8a_0^3 - 3}{10} + s(l+1/2) + 1/2\right)}.$$

Two real turning points q_- and q_+ $(Q(q_\pm) = 0)$ separate three regions.

In the first region where $0 < q < q_-$ we select the unique approximate particular logarithmic derivative $Y(q;t_0)$. In the second region where $q_- < q < q_+$ we must describe the oscillatory solution of the original Schrödinger equation (1). Therefore in this case we select two approximate particular logarithmic derivatives $Y(q;+i)$ and $Y(q;-i)$. In the third region where $q > q_+$ we must describe only the decreasing solution of the original Schrödinger equation (1). Therefore in this case we select the unique approximate particular logarithmic derivative $Y(q;0)$. Note that in the case $l = 0, s = 1$ we put $q_- = 0$.

Since the turning points are ordinary nonsingular points in our approach, no question of connection formulas arises in contrast with the conventional WKB method. Matching particular solutions at the turning points we obtain the continuous approximate radial wave function

$$\psi_{app}(r) = N_{app} r^{(s-1)/2s} \Psi_{app}(q) \tag{24}$$

where $\Psi_{app}(q)$ is represented by the following formulas

$$\Psi_1(q) = \cos\phi \exp\left(-\int_q^{q_-} Y(q';t_0)\,dq'\right) \tag{25}$$

if $0 < q < q_-$,

$$\Psi_2(q) = \exp\left(\int_{q_-}^q \frac{Y(q';+i) + Y(q';-i)}{2}\,dq'\right)\cos\left(\int_{q_-}^q \epsilon\frac{Y(q';+i) - Y(q';-i)}{2i}\,dq' - \phi\right) \tag{26}$$

if $q_- < q < q_+$,

$$\Psi_3(q) = \frac{1}{2}(-1)^n \exp\left(\int_{q_+}^q Y(q';0)\,dq'\right)\exp\left(\int_{q_-}^{q_+} \frac{Y(q';+i) + Y(q';-i)}{2}\,dq'\right) \tag{27}$$

if $q > q_+$.

Here $q = r^{1/s}, \phi = \frac{\pi}{3} - \arctan t_0, \epsilon = (dQ(q)/dq)|dQ(q)/dq|^{-1}$ and N_{app} is a normalization constant.

We have the new quantization condition

$$\int_{q_-}^{q_+} \epsilon\frac{Y(q;+i) - Y(q;-i)}{2i}\,dq = \pi(n + \frac{1}{3}) + \phi, \quad n = 0,1,2... \tag{28}$$

which determines the spectral value of E implicitly.

Note that up to now a value of s is not fixed. Numerical experiment for the power-law potentials $(k \geq 1)$ shows that the best choice for $l = 0$ is $s = 1$ and the satisfactory common choice for all $l > 0$ is $s = 2$. Thus the approximate eigenfunctions are determined completely and we can perform verification.

IV. APPLICATION TO POWER-LAW POTENTIALS

It is convenient to test our approximation with introducing the dimensionless quantities

$$x = \left(\frac{2m\alpha}{\hbar^2}\right)^{1/(k+2)} r,$$

$$e = \left(\frac{2m}{\hbar^2\alpha^{2/k}}\right)^{k(/k+2)} E.$$

Then the Schrödinger equation is rewritten in the form

$$\hat{H}\psi(x) - e\psi(x) = 0$$

with the Hamiltonian

$$\hat{H} = -\frac{d^2}{dx^2} + x^k + \frac{l(l+1)}{x^2} \qquad (29)$$

First, we estimate our approximation in the case of the harmonic oscillator potential $V(r) = \alpha r^2$ for which the exact wave functions $\psi_{ex}(x)$ are well known [11]. Figures 1, 2 and 3 show that the proposed approximation gives fairly accurate wave functions in this case. Here solid lines reproduce $\psi_{app}(x)$ and dashed lines reproduce $10(\psi_{app}(x) - \psi_{ex}(x))$. Note that without factor 10 the difference $(\psi_{app}(x) - \psi_{ex}(x))$ is invisible in comparison with $\psi_{app}(x)$.

We can calculate the expectation values

$$e_{app} = <\psi_{app}|\hat{H}|\psi_{app}> \qquad (30)$$

and

$$(e'_{app})^2 = <\psi_{app}|\hat{H}^2|\psi_{app}> \qquad (31)$$

with the help of the normalized approximate wave functions ($<\psi_{app}|\psi_{app}> = 1$). It should be stressed that $(e_{app}))^2 \neq (e'_{app})^2$ when the wave functions are not exact. Now we define the relative discrepancy

$$d = \frac{e_{app}}{e'_{app}} - 1. \qquad (32)$$

We also calculate relative virial error

$$v = \frac{<\psi_{app}| - \frac{d^2}{dx^2} + \frac{l(l+1)}{x^2}|\psi_{app}>}{<\psi_{app}|\frac{1}{2}kx^k|\psi_{app}>} - 1 \qquad (33)$$

which is equal to zero for the exact solutions. Finally, we characterize our approximation by the usual relative energy error

$$\delta e = \frac{e_{app}}{e_{ex}} - 1 \qquad (34)$$

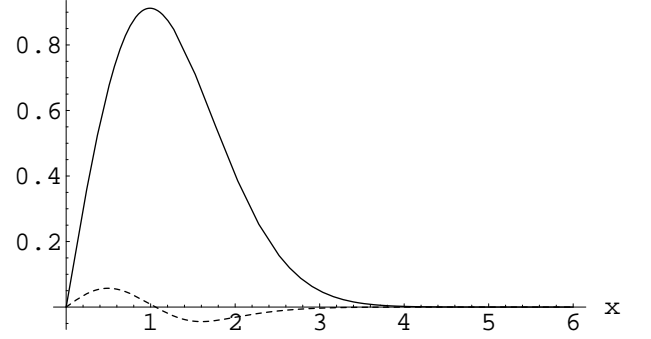where e_{ex} is the exact energy value.

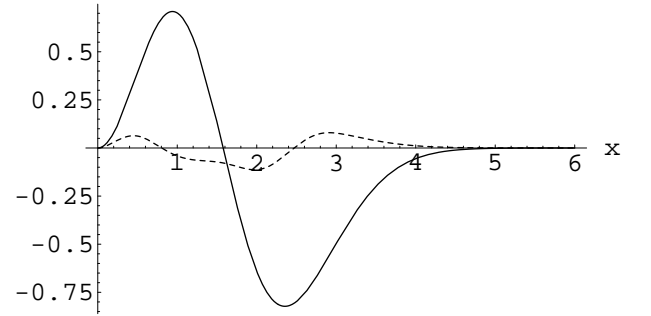FIG. 1: Harmonic oscillator radial wave function for $l = 0, n = 0$.

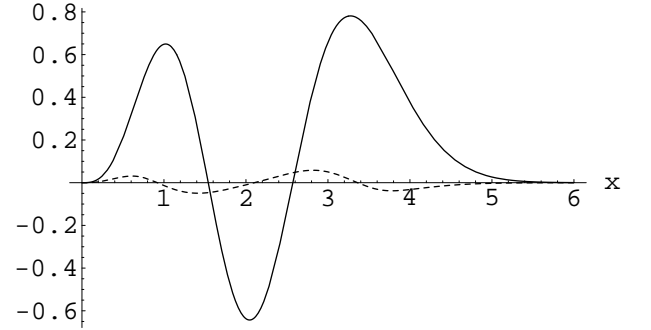FIG. 2: Harmonic oscillator radial wave function for $l = 1, n = 1$.

FIG. 3: Harmonic oscillator radial wave function for $l = 2, n = 2$.

We calculate the values δe for the linear and quartic potentials with respect to the accurate numerical eigenenergies [12]. We compare our results with the recent results in the framework of an integral semiclassical method for calculating the spectra for spherically symmetric potentials [13]. In the case of linear potential with $l = 0$ our approach gives exact eigenfunctions and eigenenergies. Table 1 demonstrates validity of our approximation in

TABLE I: Numerical verification of the proposed approximation in the case of power-law potentials $V(r) = \alpha r^k$.

l	n	v	d	e_{ex}	δe	$\delta e[13]$
			$k = 1$			
0	0	0	0	2.33811	0	$5.00 \cdot 10^{-3}$
0	1	0	0	4.08795	0	$1.50 \cdot 10^{-3}$
0	2	0	0	5.52056	0	$7.00 \cdot 10^{-4}$
1	0	$2.841 \cdot 10^{-2}$	$-3.229 \cdot 10^{-3}$	3.36126	$1.020 \cdot 10^{-3}$	$1.20 \cdot 10^{-3}$
1	1	$1.269 \cdot 10^{-2}$	$-3.563 \cdot 10^{-5}$	4.88445	$3.890 \cdot 10^{-5}$	$7.00 \cdot 10^{-4}$
1	2	$8.420 \cdot 10^{-3}$	$-2.714 \cdot 10^{-5}$	6.20762	$2.739 \cdot 10^{-5}$	$4.00 \cdot 10^{-4}$
2	0	$1.446 \cdot 10^{-2}$	$-1.607 \cdot 10^{-3}$	4.24818	$7.368 \cdot 10^{-4}$	$5.00 \cdot 10^{-4}$
2	1	$6.717 \cdot 10^{-3}$	$-7.023 \cdot 10^{-6}$	5.62971	$1.421 \cdot 10^{-5}$	$3.00 \cdot 10^{-4}$
			$k = 2$			
0	0	$1.588 \cdot 10^{-2}$	$-6.087 \cdot 10^{-5}$	3	$5.634 \cdot 10^{-5}$	–
0	1	$4.071 \cdot 10^{-3}$	$-7.104 \cdot 10^{-7}$	7	$1.889 \cdot 10^{-6}$	–
0	2	$1.939 \cdot 10^{-3}$	$-8.050 \cdot 10^{-8}$	11	$3.327 \cdot 10^{-7}$	–
1	0	$3.220 \cdot 10^{-2}$	$-9.040 \cdot 10^{-3}$	5	$1.766 \cdot 10^{-3}$	–
1	1	$1.174 \cdot 10^{-2}$	$-9.318 \cdot 10^{-5}$	9	$6.556 \cdot 10^{-5}$	–
1	2	$7.415 \cdot 10^{-3}$	$-5.584 \cdot 10^{-5}$	13	$4.615 \cdot 10^{-5}$	–
2	0	$1.614 \cdot 10^{-2}$	$-4.528 \cdot 10^{-3}$	7	$1.264 \cdot 10^{-3}$	–
2	1	$5.545 \cdot 10^{-3}$	$-2.336 \cdot 10^{-5}$	11	$2.727 \cdot 10^{-5}$	–
2	2	$3.520 \cdot 10^{-3}$	$-7.132 \cdot 10^{-6}$	15	$6.667 \cdot 10^{-6}$	–
			$k = 4$			
0	0	$2.931 \cdot 10^{-2}$	$-8.408 \cdot 10^{-4}$	3.79967	$2.543 \cdot 10^{-4}$	$-2.85 \cdot 10^{-2}$
0	1	$3.420 \cdot 10^{-3}$	$-1.627 \cdot 10^{-5}$	11.6448	$9.918 \cdot 10^{-6}$	$-5.30 \cdot 10^{-3}$
0	2	$7.311 \cdot 10^{-4}$	$-1.982 \cdot 10^{-6}$	21.2384	$1.963 \cdot 10^{-6}$	$-1.80 \cdot 10^{-3}$
1	0	$4.215 \cdot 10^{-2}$	$-2.396 \cdot 10^{-2}$	7.10845	$3.011 \cdot 10^{-3}$	$-1.00 \cdot 10^{-2}$
1	1	$1.021 \cdot 10^{-2}$	$-2.418 \cdot 10^{-4}$	16.0327	$1.185 \cdot 10^{-4}$	$-3.80 \cdot 10^{-3}$
1	2	$5.524 \cdot 10^{-3}$	$-9.617 \cdot 10^{-5}$	26.3500	$6.831 \cdot 10^{-5}$	$-1.60 \cdot 10^{-3}$
2	0	$2.090 \cdot 10^{-2}$	$-1.182 \cdot 10^{-2}$	10.8424	$2.103 \cdot 10^{-3}$	$-4.70 \cdot 10^{-3}$
2	1	$3.665 \cdot 10^{-3}$	$-8.348 \cdot 10^{-5}$	20.6435	$5.329 \cdot 10^{-5}$	$-3.00 \cdot 10^{-3}$
2	2	$1.630 \cdot 10^{-3}$	$-1.928 \cdot 10^{-5}$	31.6147	$1.265 \cdot 10^{-5}$	$-1.70 \cdot 10^{-3}$

the linear, quadratic and quartic cases .

V. CONCLUSION

An old problem in semiclassical analysis is the development of global uniform approximations for the wave functions. In the present paper, this problem has been solved by means of the reconstruction of the WKB series and subsequent explicit summation of the leading constituent (partial) series. Such approach yields satisfactory description of the wave functions in the important case of the radial Schrödinger equation with the power-law potentials.

[1] R. E. Langer. On the connection formulas and the solutions of the wave equation. Phys. Rev. **51**, no. 8, 669-676 (1937).

[2] J. B. Krieger, C. Rosenzweig. Application of a higher-order WKB approximation to radial problems. Phys. Rev. **164**, no. 1, 171-173 (1967).

[3] N. Fröman, P. O. Fröman. *Phase-Integral Method: Allowing Nearlying Transition Points* (Springer-Verlag, New York, 1996).

[4] M. Seetharaman, S. S. Vasan. Energy eigenvalues of d-dimensional quartic oscillator. J. Math. Phys. **27**, no. 4, 1031-1036 (1986).

[5] M. Lakshmanan *et al.* Phase-integral approach to quantal two- and three-dimensional isotropic oscillator. Phys. Rev. A **49**, no. 5, 3296-3309 (1994).

[6] C. M. Bender, K. Olaussen, P. S. Wang. Numerological analysis of the WKB approximation in large order. Phys. Rev. D **16**, no. 6, 1740-1748 (1977).

[7] C. M. Bender, S. A. Orszag. *Advanced Mathematical Methods for Scientists and Engineers* (McGraw-Hill, New

York, 1978).

[8] V. V. Kudryashov. Reconstruction of the WKB series as a new method for the approximate solution of the Schrödinger equation. Doklady of the National Academy of Sciences of Belarus **42**, no. 6, 45-49 (1998) (in Russian).

[9] V. V. Kudryashov, Yu. V. Vanne. Explicit summation of the constituent WKB series and new approximate wave functions. J. Appl. Math. **2**, no. 6, 265-275 (2002).

[10] M. Abramovitz, I. A. Stegun (eds.). *Handbook of Mathematical Functions* (Dover Publications, New York,

1970).

[11] S. Flügge. *Practical Quantum Mechanics* (Springer-Verlag, Berlin, 1999).

[12] B. M. Karnakov, V. D. Mur, V. S. Popov. On the matching condition in the WKB method. Zh. Eks. Teor. Fiz. (JETP) **107**, no. 6, 1768-1779 (1995).

[13] A. A. Lobashev, N. N. Trunov. An integral semiclassical method for calculating the spectra for centrally symmetric potentials. Theor. Math. Phys. **124**, no. 3, 1250-1264 (2000).